THE COMPUTER AT THE END OF THE RAINBOW

"In the past 50 years, computer performance has improved an average of 60 percent every year. So computers are 100 billion times better than in the days of Atanasoff. That's in one lifetime. A factor of 100 billion in one lifetime."

-John Gustafson
Ames Lab Computational Scientist

The race for better computers is a marathon: the competitors have been at it for 50 years, and the finish line is nowhere in sight. But no one really cares about the finish line, because merely taking a lead in this race produces abundant rewards.

“High-performance computing is a very important tool for industrial design, manufacturing, preservation of the environment and so on,” says David Nelson, acting associate director of Energy Research for the Department of Energy’s (DOE) Office of Scientific Computing. “Any nation that can accelerate the development and application of high-performance computing is going to receive a payoff in goods and services that are cheaper, faster, more competitive worldwide, and have less impact on the environment.”

Ames Laboratory is an active contributor to U.S. efforts to maintain an edge on other nations in high-performance computing. Through the Department of Energy’s Partnership in Computational Science, a program under the federal government’s High Performance Computing and Communications (HPCC) program, Ames Lab is applying its expertise in computer evaluation, materials sciences and science education to help advance the use of high-speed computers in the United States.

Tests rate computers abilities

At the Lab’s Scalable Computing Laboratory (SCL), scientists are developing better methods for rating the performance of supercomputers. John Gustafson, director of the SCL and an Iowa State University (ISU) adjunct professor of computational science, explains that improved rating systems will help the United States on two fronts, allowing policy-makers to decide which advanced computer designs are worth investing in and helping scientists decide what computer system will best fulfill their particular research needs.

Two years ago, Gustafson and a team of Lab researchers developed SLALOM, a prize-winning computer benchmark that has received widespread acceptance among computer manufacturers. Through the Partnership, they are continuing to improve and further develop SLALOM, but Gustafson has also set some members of his team working on a more ambitious goal.

“We’re hoping to finally come up with a system that can be read off the label, something almost as simple as a miles-per-gallon rating for a car or a voltage rating for a battery,” says Gustafson. “We’d like to keep it almost that simple and, hopefully, almost as accurate.”

On another front, the facility's computer researchers are searching for shortcuts in programming and problem-solving techniques that will let scientists more effectively use limited computer time.

"You'd be surprised—a guy on foot can sometimes beat a Ferrari just by knowing a few of the right shortcuts," Gustafson explains. "Sometimes we find spectacular shortcuts. It's impossible to do this on demand, though, so we just try to keep our eyes open."

New computer part of Partnership

Through the partnership, the SCL is scheduled to receive a Paragon, a new parallel supercomputer, in April. The Paragon will have 28 processors, each capable of about 20 megaflops (millions of floating point operations per second). Each processor can work on one portion of the problem while other processors work at the same time on different portions of the problem, solving the entire problem in a shorter period of time.

"Our Paragon will be compatible with the Paragon at Oak Ridge National Laboratory, which has 512 processors and is, by some measures, the fastest computer currently available," says Gustafson.

Other programs at the Lab will access the Paragon; in particular, the Paragon will give condensed matter physicists and materials scientists at Ames Laboratory more opportunities to work on their components of the Partnership, according to Bruce Harmon, director of the Lab's condensed Matter Physics program and a professor of physics at ISU.

Harmon says researchers in the program will be working to fully utilize the advantages offered by parallel computers: developing new problem-solving techniques specifically for parallel computers and transforming the computer models and simulations that they already use into programs that will run well on parallel computers.

"The big issue for us is learning how to take a program that runs well on a serial computer and efficiently split that up into individual tasks for a number of different processors," he says.

In the past, Harmon points out, materials scientists have concentrated on more approximate models and techniques that deal with thousands of atoms as large structures, while physicists like Harmon have focused their research on highly precise techniques dealing with a few atoms.

"There are, however, a number of problems in condensed matter physics and materials sciences where the scale of interactions or phenomena are larger than just a few atoms," Harmon says. "Examples include dislocations, magnetic domains and lattice relaxations around impurities."

Highly accurate studies of hundreds or thousands of atoms would have taken too much time on serial computers; parallel computers can handle them in an acceptable amount of time, allowing physicists and materials scientists to meet at a new middle ground.

"These machines will allow physicists to interact with materials designers, engineers and others in a way that we have never before been able to," Harmon concludes.

An integrated effort

The other component of Ames Laboratory's work for the Partnership is the Adventures in Supercomputing (AIS) program, which encourages interest in science and math among high school students. AIS is administered by the Lab's Applied Mathematical Sciences program and helps teachers hook their classrooms up to and run experiments on a Lab supercomputer.

Jim Corones, director of the Lab's math program, emphasizes that all of the Lab's work for the Partnership is an integrated effort, both within the Lab and with the other laboratories in the Partnership. Oak Ridge National Laboratory in Oak Ridge, TN, coordinates the partnership; Brookhaven National Laboratory of Long Island, NY, and Sandia National Laboratory of Albuquerque, NM, are also participants, as are a number of major research universities.

Integrating research at the Lab is relatively easy, John Gustafson explains, noting that his research team regularly interfaces with scientists in the condensed matter physics and the AIS educational programs.

"This is a small lab," Gustafson says. "We don't have to work all that hard to make an interface happen. Somebody walks over to another building and asks a question. That's how the interface works."